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On the necessity of negative coefficients for operator splitting schemes of order higher than two

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Abstract

In this paper we analyse numerical integration methods applied to differential equations which are separable in solvable parts. These methods are compositions of flows associated with each part of the system. We propose an elementary proof of the necessary existence of negative coefficients if the schemes are of order, or effective order, $p \geqslant 3$ and provide additional information about the distribution of these negative coefficients. It is shown that if the methods involve flows associated with more general terms this result does not necessarily apply and in some cases it is possible to build higher order schemes with positive coefficients.

Keywords: Splitting methods; Composition methods; Effective order; Numerical integrators

1. Introduction

Operator splitting schemes are numerical methods which are particularly useful to approximate the evolution of differential equations when they are separable in solvable parts [17]. To be more specific, let us consider the ODE

$$x' = f(x), \quad x_0 = x(0) \in \mathbb{R}^D \tag{1}$$

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with $f:\mathbb{R}^D \to \mathbb{R}^D$ and associated vector field (or Lie operator associated with f)

$$F=\sum_{i=1}^{D} f_i(x)\frac{\partial}{\partial x_i}. \tag{2}$$

Let us denote by φ_h the h-flow of the ODE (1) for a given time step h. In other words, the exact solution is given by $x(h)=\varphi_h(x_0)$.

Now let us assume that $f(x)$ can be written as $f(x)=f_A(x)+f_B(x)$, the vector field F is split accordingly as $F=F_A+F_B$ and the h-flows $\varphi_h^{[A]}$ and $\varphi_h^{[B]}$ corresponding to F_A and F_B, respectively, can be exactly computed or, equivalently, the equations $x'=f_A(x)$ and $x'=f_B(x)$ are solvable. Then the composition (sometimes called Lie–Trotter splitting)

$$\psi_{h,1}\equiv\varphi_h^{[B]}\circ\varphi_h^{[A]} \tag{3}$$

approximates φ_h with error of order h^2, i.e., $\psi_{h,1}(x_0)=\varphi_h(x_0)+\mathcal{O}(h^2)$, whereas the so-called Strang splitting or Störmer/Verlet/leapfrog scheme

$$\psi_{h,2}\equiv\varphi_{h/2}^{[A]}\circ\varphi_h^{[B]}\circ\varphi_{h/2}^{[A]} \tag{4}$$

is such that $\psi_{h,2}(x_0)=\varphi_h(x_0)+\mathcal{O}(h^3)$. The order of approximation to the exact solution can be increased by including more maps with fractional time steps in the composition. In general, the scheme

$$\psi_h\equiv\varphi_{b_m h}^{[B]}\circ\varphi_{a_m h}^{[A]}\circ\cdots\circ\varphi_{b_1 h}^{[B]}\circ\varphi_{a_1 h}^{[A]}, \tag{5}$$

$(a_1,b_1,\ldots,a_m,b_m)\in\mathbb{R}^{2m}$, is of order p if $\psi_h=\varphi_h+\mathcal{O}(h^{p+1})$ for a proper choice of m and coefficients a_i, b_i. It can be assumed without loss of generality that in (5) none of the coefficients $b_1,b_2,\ldots,b_{m-1}$ as well as none of $a_2,a_3,\ldots,a_m$ are vanishing, i.e., only a_1 and/or b_m can be zero, since otherwise the corresponding flows could be removed ($\varphi_0^{[A]}=\varphi_0^{[B]}=\mathrm{id}$, the identity map) and the rest of the maps would be concatenated (due to the group property of the flows).

Numerical schemes of order $p\geqslant 3$ based on the composition (5) have been successfully applied for solving a large number of problems [10,17], including also certain partial differential equations. In fact, splitting methods are frequently used in celestial mechanics [21], quantum mechanics [6], molecular dynamics [12], accelerator physics [7] and, in general, for numerically solving Hamiltonian dynamical systems [8,16], Poisson systems [14] and reversible differential equations [15]. It has been noticed, however, that some of the coefficients in (5) are negative for $p\geqslant 3$ when one considers arbitrary vector fields F_A and F_B. In other words, the methods always involve stepping backwards in time. This constitutes a problem when the differential equation is defined in a semigroup, as arises sometimes in applications, since then the method can only be conditionally stable [17]. Also schemes with negative coefficients may not be well-posed when applied to PDEs involving unbounded operators.

The existence of backward fractional time steps in the composition method (5) is in fact unavoidable, and can be established as the following two theorems:

Theorem 1 [20,22]. *If p is a positive integer such that $p\geqslant 3$, then there are no composition methods of the form* (5) *and finite m with all the coefficients a_i, b_i being positive.*

Theorem 2 [9]. *If p is a positive integer such that $p\geqslant 3$, then, for every pth-order method* (5) *with m any finite positive integer, one has*

$$\min_{1\leqslant i\leqslant m} a_i<0 \quad \textit{and} \quad \min_{1\leqslant j\leqslant m} b_j<0.$$

Theorem 2 is stronger than Theorem 1, in the sense that it establishes that at least one of the a_i *and* also one of the b_i coefficients have to be strictly negative, although a similar (and certainly non-trivial) proof strategy was used. One of the goals of this paper is to provide an alternative, elementary proof of Theorem 2, giving in addition a more detailed analysis of how negative coefficients are distributed in the composition.

During the last few years the processing technique has been used to find composition methods requiring less evaluations than conventional schemes of order p [13]. The idea consists in enhancing an integrator ψ_h (the *kernel*) with a parametric map $\pi_h : \mathbb{R}^D \to \mathbb{R}^D$ (the *post-processor*) as

$$\hat{\psi}_h = \pi_h \circ \psi_h \circ \pi_h^{-1}. \tag{6}$$

Application of n steps of the new (and hopefully better) integrator $\hat{\psi}_h$ leads to

$$\hat{\psi}_h^n = \pi_h \circ \psi_h^n \circ \pi_h^{-1},$$

which can be considered as a change of coordinates in phase space. Observe that processing is advantageous if $\hat{\psi}_h$ is a more accurate method than ψ_h and the cost of π_h is negligible, since it provides the accuracy of $\hat{\psi}_h$ at essentially the cost of the least accurate method ψ_h.

The simplest example of a processed integrator is provided in fact by the Strang splitting (4). As a consequence of the group property of the exact flow, we have

$$\begin{aligned} \psi_{h,2} &= \varphi_{h/2}^{[A]} \circ \varphi_h^{[B]} \circ \varphi_{h/2}^{[A]} = \varphi_{h/2}^{[A]} \circ \varphi_h^{[B]} \circ \varphi_h^{[A]} \circ \varphi_{-h}^{[A]} \circ \varphi_{h/2}^{[A]} \\ &= \varphi_{h/2}^{[A]} \circ \psi_{h,1} \circ \varphi_{-h/2}^{[A]} = \pi_h \circ \psi_{h,1} \circ \pi_h^{-1} \end{aligned} \tag{7}$$

with $\pi_h = \varphi_{h/2}^{[A]}$. Hence, applying the first order method (3) with processing yields a second order of approximation.

Although initially intended for Runge–Kutta methods [4], the processing technique has proved its usefulness mainly in the context of geometric numerical integration [10], where constant step-sizes are widely employed.

We say that the method ψ_h is of *effective order* p if a post-processor π_h exists for which $\hat{\psi}_h$ is of (conventional) order p [4], that is,

$$\pi_h \circ \psi_h \circ \pi_h^{-1} = \varphi_h + \mathcal{O}(h^{p+1}).$$

Hence, as the previous example shows, the Lie–Trotter splitting (3) is of effective order 2. Obviously, a method of order p is also of effective order p (taking $\pi_h = \mathrm{id}$) or higher, but the converse is not true in general.

The analysis of the order conditions of the method $\hat{\psi}_h$ shows that many of them can be satisfied by π_h, so that ψ_h must fulfill a much reduced set of restrictions [2,3]. In particular, if one takes a composition (5) for ψ_h, the number and complexity of the conditions to be verified by the coefficients a_i, b_i is notably reduced. As a consequence, by considering both the kernel ψ_h and the post-processor π_h as compositions of basic integrators, highly efficient processed methods have been proposed [23,2,1,17]. Nevertheless, when π_h is constructed as a composition (5), its computational cost is usually higher than that of ψ_h, and thus the use of the resulting processed scheme is restricted to situations where intermediate results are not frequently required. Otherwise the overall efficiency of the method is deteriorated.

To overcome this difficulty, in [3] a technique has been developed for obtaining approximations to the post-processor at virtually cost free and without loss of accuracy. The clue is to replace π_h by a new integrator $\tilde{\pi}_h \simeq \pi_h$ obtained from the intermediate stages in the computation of ψ_h. As a result of the analysis carried out in [3], it is generally recommended to have a very accurate pre-processor π_h^{-1} but, on the contrary, π_h can safely be replaced by $\tilde{\pi}_h$, since the error introduced by the cheap approximation $\tilde{\pi}_h$ is of a purely local character and is not propagated along the evolution (contrarily to the error in π_h^{-1}).

Here we also address the following question: do Theorems 1 and 2 also hold for a composition ψ_h of effective order $p \geqslant 3$? Observe that, in principle, Theorem 2 applies to the whole composition $\hat{\psi}_h$ of (6), but it would nonetheless be advantageous to have the negative coefficients restricted only to the composition π_h. For in that case the integration starts by computing π_h^{-1} (which only involves positive coefficients), then ψ_h (involving only positive coefficients) is evaluated once per step and finally an appropriate approximation to π_h may be considered when output is required (even the crudest approximation $\pi_h = \mathrm{id}$ [13]). In this way the algorithm only involves stepping forward in time and could be applied even to PDEs with unbounded operators. The answer to the question posed before could also be useful in the search of efficient methods of order higher than 2 for systems that evolve in a semigroup, such as the heat equation in two space dimensions [17].

Also in quantum statistical mechanics, the partition function requires computing $Z = \mathrm{Tr}(\mathrm{e}^{-\beta H})$, where H is the Hamiltonian operator and β is the inverse temperature [22]. In numerical calculations a processed composition algorithm may be used to approximate $\mathrm{e}^{-\beta H}$, and since the trace is invariant under similarity transformations, only the kernel is necessary to determine Z. If it involves only positive coefficients then it would be possible to build up higher order convergent algorithms for this class of problems.

In Section 3 we prove explicitly that this is not the case, so that any composition method (5) of effective order $p \geqslant 3$ contains necessarily some negative coefficients.

2. An elementary proof of Theorem 2

It is well known that, for each infinitely differentiable map $g : \mathbb{R}^D \to \mathbb{R}$, $g(\varphi_h(x))$ admits an expansion of the form

$$g\big(\varphi_h(x)\big) = g(x) + \sum_{k\geqslant 1} \frac{h^k}{k!} F^k[g](x) = \mathrm{e}^{hF}[g](x), \qquad x \in \mathbb{R}^D,$$

where F is the vector field (2). Similarly, for the map ψ_h given in (5) one has

$$g\big(\psi_h(x)\big) = \Psi_h[g](x),$$

where [10]

$$\Psi_h = \exp(ha_1 F_A)\, \exp(hb_1 F_B) \cdots \exp(ha_m F_A)\, \exp(hb_m F_B). \tag{8}$$

By repeated application of the Baker–Campbell–Hausdorff (BCH) formula to (8) we can obtain a series of differential operators $F_h = \sum_{k\geqslant 1} h^k F_k$ such that $\Psi_h = \exp(F_h)$, i.e., ψ_h is formally the exact 1-flow of the vector field F_h. The scheme ψ_h is of order $p \geqslant 3$ if $F_1 = F_A + F_B$ and $F_2 = F_3 = 0$. In terms of the coefficients a_i, b_i, this corresponds to the following order conditions:

$$\text{order 1:} \qquad \sum_{i=1}^{m} a_i = 1, \qquad \sum_{i=1}^{m} b_i = 1;$$
$$\text{order 2:} \qquad \sum_{i=1}^{m} b_i \left(\sum_{j=1}^{i} a_j \right) = \frac{1}{2};$$
$$\text{order 3:} \qquad \sum_{i=1}^{m-1} b_i \left(\sum_{j=i+1}^{m} a_j \right)^2 = \frac{1}{3}, \qquad \sum_{i=1}^{m} a_i \left(\sum_{j=i}^{m} b_j \right)^2 = \frac{1}{3}. \tag{9}$$

The proof of Theorems 1 and 2 provided by [20,22,9] is based precisely on the fact that a scheme of the form (5) with m any finite positive integer and all the coefficients a_i, b_i being positive cannot satisfy Eqs. (9).

In the particular case of the first order method $\chi_h = \varphi_h^{[B]} \circ \varphi_h^{[A]}$, the corresponding operator (8) is given by

$$\exp(hF_A)\exp(hF_B) = \exp(X_h) = \exp\bigl(hX_1 + h^2X_2 + h^3X_3 + \cdots\bigr), \tag{10}$$

with $X_1 = F_A + F_B$, $X_2 = \frac{1}{2}[F_A, F_B]$, etc., whereas for its adjoint scheme $\chi_h^* = \chi_{-h}^{-1} = \varphi_h^{[A]} \circ \varphi_h^{[B]}$ one has $g(\chi_h^*(x)) = \mathrm{e}^{-X_{-h}}[g](x)$. Here $[F_A, F_B]$ stands for the Lie bracket $F_AF_B - F_BF_A$. Since our aim is to get results valid for all pairs F_A, F_B of arbitrary vector fields, then we must assume that the only linear dependencies among nested Lie brackets of F_A and F_B can be derived from the skew-symmetry and the Jacobi identity of the Lie brackets. In other words, X_k, $k \geqslant 1$, is an element of the graded free Lie algebra generated by the symbolic vector fields F_A, F_B, where both have degree one [18].

The crucial observation that leads to an alternative, elementary proof of Theorem 2 is the close connection existing between the splitting method (5)

$$\psi_h = \varphi_{b_m h}^{[B]} \circ \varphi_{a_m h}^{[A]} \circ \varphi_{b_{m-1} h}^{[B]} \circ \cdots \circ \varphi_{a_2 h}^{[A]} \circ \varphi_{b_1 h}^{[B]} \circ \varphi_{a_1 h}^{[A]} \tag{11}$$

and the composition of the first order method $\chi_h = \varphi_h^{[B]} \circ \varphi_h^{[A]}$ and its adjoint $\chi_h^* = \varphi_h^{[A]} \circ \varphi_h^{[B]}$ with different time steps [15]:

$$\psi_h = \chi_{\beta_{2m} h}^* \circ \chi_{\beta_{2m-1} h} \circ \cdots \circ \chi_{\beta_2 h}^* \circ \chi_{\beta_1 h} \circ \chi_{\beta_0 h}^*. \tag{12}$$

Indeed, by inserting the explicit form of $\chi_{\beta_i h}$ and $\chi_{\beta_i h}^*$ in (12) we have

$$\begin{aligned} \psi_h &= \bigl(\varphi_{\beta_{2m} h}^{[A]} \circ \varphi_{\beta_{2m} h}^{[B]}\bigr) \circ \bigl(\varphi_{\beta_{2m-1} h}^{[B]} \circ \varphi_{\beta_{2m-1} h}^{[A]}\bigr) \circ \cdots \circ \bigl(\varphi_{\beta_2 h}^{[A]} \circ \varphi_{\beta_2 h}^{[B]}\bigr) \circ \bigl(\varphi_{\beta_1 h}^{[B]} \circ \varphi_{\beta_1 h}^{[A]}\bigr) \circ \bigl(\varphi_{\beta_0 h}^{[A]} \circ \varphi_{\beta_0 h}^{[B]}\bigr) \\ &= \varphi_{\beta_{2m} h}^{[A]} \circ \varphi_{(\beta_{2m}+\beta_{2m-1})h}^{[B]} \circ \varphi_{(\beta_{2m-1}+\beta_{2m-2})h}^{[A]} \circ \cdots \circ \varphi_{(\beta_2+\beta_1)h}^{[B]} \circ \varphi_{(\beta_1+\beta_0)h}^{[A]} \circ \varphi_{\beta_0 h}^{[B]}, \end{aligned}$$

where in the last equality we have used the group property of the exact flow. If we put $\beta_0 = \beta_{2m} = 0$ we recover expression (11) as soon as

$$a_i = \beta_{2i-1} + \beta_{2i-2}, \qquad b_i = \beta_{2i} + \beta_{2i-1}, \quad i = 1, \ldots, m. \tag{13}$$

Then

$$\sum_{i=1}^{m} a_i = \sum_{i=0}^{2m} \beta_i = \sum_{i=1}^{m} b_i. \tag{14}$$

In consequence, composition (11) can be rewritten as (12) only if (14) holds. Consistency of both schemes require in fact that $\sum_{i=1}^{m} a_i = \sum_{i=1}^{m} b_i = \sum_{i=0}^{2m} \beta_i = 1$ and it has been shown in [15] that the order conditions for the coefficients a_i, b_i to get a method of order $p \geqslant 1$ are equivalent to the order conditions for the β_i. In that case the operator Ψ_h given in (8) can also be expressed as

$$\Psi_h = \exp(-X_{-\beta_0 h}) \exp(X_{\beta_1 h}) \exp(-X_{-\beta_2 h}) \cdots \exp(X_{\beta_{2m-1} h}) \exp(-X_{-\beta_{2m} h}) \tag{15}$$

and repeated application of the BCH formula gives

$$\Psi_h = \exp\bigl(h f_{1,1} X_1 + h^2 f_{2,1} X_2 + h^3 \bigl(f_{3,1} X_3 + f_{3,2}[X_1, X_2]\bigr) + \mathcal{O}\bigl(h^4\bigr)\bigr),$$

where the coefficients $f_{k,j}$ are homogeneous polynomials of degree k in the variables β_i. In particular we have

$$f_{1,1} = \sum_{i=0}^{2m} \beta_i, \qquad f_{2,1} = \sum_{i=0}^{2m} (-1)^{i+1} \beta_i^2, \qquad f_{3,1} = \sum_{i=0}^{2m} \beta_i^3. \tag{16}$$

Conditions $f_{1,1} = 1$ and $f_{n,j} = 0$ for all $n \leqslant p$ are then sufficient for the method to be of order p.

Proof of Theorem 2. From the preceding discussion, it is clear that

$$f_{3,1} = \sum_{i=0}^{2m} \beta_i^3 = 0 \tag{17}$$

is a necessary condition to be satisfied by any method of order $p \geqslant 3$. We suppose that more than two β_i are different from zero because $\beta_1^3 + \beta_2^3 = 0$ together with the consistency condition $\beta_1 + \beta_2 = 1$ have no real solution. Now (17) can be written as

$$\sum_{i=1}^{m} \bigl(\beta_{2i-1}^3 + \beta_{2i-2}^3\bigr) + \beta_{2m}^3 = \sum_{i=1}^{m} \bigl(\beta_{2i-1}^3 + \beta_{2i-2}^3\bigr) = 0,$$

for any positive integer m. In consequence $\beta_{2j-1}^3 + \beta_{2j-2}^3$ has to be negative for some $1 \leqslant j \leqslant m$. But it is easy to verify that $\operatorname{sign}(x^3 + y^3) = \operatorname{sign}(x + y)$ for any $x, y \in \mathbb{R}$, so that

$$a_j = \beta_{2j-1} + \beta_{2j-2} < 0, \tag{18}$$

for some j such that $1 \leqslant j \leqslant m$. Similarly, we can write (17) as

$$\beta_0^3 + \sum_{i=1}^{m} \bigl(\beta_{2i}^3 + \beta_{2i-1}^3\bigr) = \sum_{i=1}^{m} \bigl(\beta_{2i}^3 + \beta_{2i-1}^3\bigr) = 0$$

so that $\beta_{2k}^3 + \beta_{2k-1}^3 < 0$ for some $1 \leqslant k \leqslant m$, and again

$$b_k = \beta_{2k} + \beta_{2k-1} < 0. \qquad \square \tag{19}$$

Distribution of the coefficients

We can get more information about the distribution of the negative coefficients in the composition (5) by applying a slightly more involved argument which, in fact, also provides another demonstration of Theorem 2.

If we denote $\alpha_{2i-1} = a_i$, $\alpha_{2i} = b_i$, $i = 1, \ldots, m$, in the composition (5)

$$\psi_h = \varphi^{[B]}_{\alpha_{2m}h} \circ \varphi^{[A]}_{\alpha_{2m-1}h} \circ \cdots \circ \varphi^{[B]}_{\alpha_2 h} \circ \varphi^{[A]}_{\alpha_1 h},$$

then (13) implies

$$\alpha_i = \beta_i + \beta_{i-1}, \quad i = 1, \ldots, 2m, \tag{20}$$

where β_j are the coefficients appearing in (12) ($\beta_0 = \beta_{2m} = 0$). Now all we need to prove Theorem 2 is to analyse how Eqs. (17) and (20) imply that at least one odd as well as one even α_i coefficients are negative.

As before, we assume that there are more than two nonvanishing coefficients β_i and at least one of them is negative.

(a) Let us suppose first that only one coefficient is actually negative, say β_j, for some $0 < j < 2m$. Then, from Eq. (17),

$$\beta_j = -\Big(\sum_{i\neq j} \beta_i^3\Big)^{1/3}$$

so that $|\beta_j| > \beta_i$ for all $i \neq j$. Therefore

$$\alpha_j = \beta_j + \beta_{j-1} < 0 \quad \text{and} \quad \alpha_{j+1} = \beta_{j+1} + \beta_j < 0,$$

i.e., two consecutive α_k coefficients are negative, and thus at least one a_j and one b_j are negative.

(b) Suppose now that the negative coefficients are $\beta_{j_1}, \beta_{j_2}, \ldots, \beta_{j_k}$ with $j_1 < j_2 < \cdots < j_k$.

(b.1) If

$$\beta_{j_i-1} < |\beta_{j_i}| \quad \text{and} \quad |\beta_{j_i}| > \beta_{j_i+1} \tag{21}$$

for some $j_i \in \mathcal{I} \equiv \{j_1, j_2, \ldots, j_k\}$ then also two consecutive coefficients α_k are negative, namely α_{j_i} and α_{j_i+1}.

(b.2) On the other hand, when (21) does not hold for any $j_i \in \mathcal{I}$, then the following situations are possible:

(i) if $\beta_{j_i-1} < |\beta_{j_i}|$, then $|\beta_{j_i}| < \beta_{j_i+1}$;
(ii) if $|\beta_{j_i}| > \beta_{j_i+1}$, then $\beta_{j_i-1} > |\beta_{j_i}|$;
(iii) finally, $\beta_{j_i-1} > |\beta_{j_i}|$ and $\beta_{j_i+1} > |\beta_{j_i}|$.

Let us suppose that $\beta_{j_i+1} \neq \beta_{j_{i+1}-1}$ for all j_i. Then

$$\begin{aligned}\beta_{j_k} = -\Big(&\big(\beta^3_{j_1-1} + \beta^3_{j_1} + \beta^3_{j_1+1}\big) + \big(\beta^3_{j_2-1} + \beta^3_{j_2} + \beta^3_{j_2+1}\big) + \cdots \\ &+ \big(\beta^3_{j_{k-1}-1} + \beta^3_{j_{k-1}} + \beta^3_{j_{k-1}+1}\big) + \sum{}' \beta_i^3\Big)^{1/3},\end{aligned}$$

where $\sum'$ contains the remaining terms (including β_{j_k-1} and β_{j_k+1}). Since $\beta^3_{j_l-1} + \beta^3_{j_l} + \beta^3_{j_l+1} > 0$ for $l = 1, \ldots, k-1$, then clearly

$$|\beta_{j_k}| > \beta_{j_k-1} \quad \text{and} \quad |\beta_{j_k}| > \beta_{j_k+1}$$

in contradiction with hypothesis (b.2). Therefore $\beta_{j_i+1} = \beta_{j_{i+1}-1}$ for some j_i. Let us suppose, without loss of generality, that they correspond to the first $l+1$ coefficients β_{j_i}. Then, the only possible sequence (different from those considered before) has to be $\beta_{j_i-1}, \beta_{j_i}, \beta_{j_i+1}, \beta_{j_i+2}, \beta_{j_i+3}, \dots, \beta_{j_i+2l-1}, \beta_{j_i+2l}, \beta_{j_i+2l+1}$ such that

$$\begin{aligned} &\beta_{j_i-1} < |\beta_{j_i}| < \beta_{j_i+1}, \\ &|\beta_{j_i+2}| < \beta_{j_i+1}, \qquad |\beta_{j_i+2}| < \beta_{j_i+3}, \quad \dots \\ &\beta_{j_i+2l-1} > |\beta_{j_i+2l}| > \beta_{j_i+2l+1}, \end{aligned}$$

where β_{j_i+2k}, $k = 0, 1, \dots, l$ are the negative coefficients. Then

$$\alpha_{j_i} = \beta_{j_i} + \beta_{j_i-1} < 0, \qquad \alpha_{j_i+2l+1} = \beta_{j_i+2l+1} + \beta_{j_i+2l} < 0.$$

Also in this case at least one a_i and one b_i are negative because j_i and $j_i + 2l + 1$ differ in an odd number.

Notice that this is the only situation where two negative α_i coefficients in a given method do not stay in consecutive places. We have checked several composition methods published in the literature having observed that this occurrence is in fact quite rare: it is very much frequent that at least two consecutive α_i coefficients are negative, and this discussion provides an explanation of the phenomenon.

3. Compositions of effective order $p \geqslant 3$

As with the composition ψ_h in (5), let us consider a post-processor π_h in (6) formally as the exact 1-flow of the vector field P_h, i.e., $g(\pi_h(x)) = \mathrm{e}^{P_h}[g](x)$ for all g, with $P_h = \sum_{k\geqslant 1} h^k P_k$. Then one has for the processed scheme $g \circ \hat{\psi}_h = \widehat{\Psi}_h[g]$, where $\widehat{\Psi}_h = \exp(\widehat{F}_h)$ and the vector field $\widehat{F}_h$ can be determined from the relation

$$\exp\bigl(\widehat{F}_h\bigr) = \exp(-P_h)\exp(F_h)\exp(P_h). \tag{22}$$

With respect to the vector field P_h, it is natural to choose it as an element of the graded free Lie algebra generated by F_A and F_B. Thus, up to order two in h,

$$P_h = h(c_1 F_A + c_2 F_B) + h^2 c_3 X_2 + \mathcal{O}\bigl(h^3\bigr), \tag{23}$$

with c_i free parameters. Notice that π_h can be approximated by a composition (5), or equivalently, $\exp(P_h)$ by the product (8). However, if $c_1 \neq c_2$ then $\sum_i a_i = c_1 \neq c_2 = \sum_i b_i$ and composition (12) cannot be used (as is the case, for instance, of the Strang splitting (7)). On the other hand, since $c_1 F_A + c_2 F_B = (c_2 - c_1) F_B + c_1 X_1 = (c_1 - c_2) F_A + c_2 X_1$, from (23) it is possible to write

$$\mathrm{e}^{P_h} = \mathrm{e}^{hc_1 X_1} \mathrm{e}^{hcF_B} \mathrm{e}^{h^2 d_1 X_2} + \mathcal{O}\bigl(h^3\bigr) \tag{24}$$

as well as

$$\mathrm{e}^{P_h} = \mathrm{e}^{hc_2 X_1} \mathrm{e}^{-hcF_A} \mathrm{e}^{h^2 d_2 X_2} + \mathcal{O}\bigl(h^3\bigr), \tag{25}$$

where $c = c_2 - c_1$ and d_1, d_2 are parameters depending on c_1, c_2, c_3. Since the processed scheme $\hat{\psi}_h$ is of conventional order p, then $\widehat{\Psi}_h = \exp(hX_1) + \mathcal{O}(h^{p+1})$ and $\mathrm{e}^{hX_1}\widehat{\Psi}_h = \widehat{\Psi}_h \mathrm{e}^{hX_1} + \mathcal{O}(h^{p+1})$, so that $\exp(hc_i X_1)$ in (24) and (25) can be safely removed without loss of generality and thus we take $c_1 = 0$ or $c_2 = 0$.

Now we are in disposition to establish and prove the main result of this section.

Theorem 3. *At least one of the a_i as well as one of the b_i coefficients have to be negative in the composition* (5) *if ψ_h is the kernel of a processed method of order* (*or equivalently if ψ_h is of effective order*) $p \geqslant 3$.

Proof. Let ψ_h be a composition (5) of effective order 3 with, say, all a_i positive. Then it is possible to construct a vector field P_h such that (24) (with $c_1 = 0$) holds and therefore (22) leads to

$$\mathrm{e}^{-h^2 d_1 X_2} \mathrm{e}^{-hcF_B} \Psi_h \mathrm{e}^{hcF_B} \mathrm{e}^{h^2 d_1 X_2} = \mathrm{e}^{\widehat{F}_h} = \mathrm{e}^{h(F_A+F_B)} + \mathcal{O}\big(h^4\big), \tag{26}$$

or equivalently

$$\begin{aligned}\overline{\Psi}_h \equiv \mathrm{e}^{-hcF_B} \Psi_h \mathrm{e}^{hcF_B} &= \mathrm{e}^{h^2 d_1 X_2} \mathrm{e}^{h(F_A+F_B)} \mathrm{e}^{-h^2 d_1 X_2} + \mathcal{O}\big(h^4\big) \\ &= \exp\big(h(F_A + F_B) - h^3 d_1 [X_1, X_2]\big) + \mathcal{O}\big(h^4\big),\end{aligned} \tag{27}$$

where Ψ_h is given by (8). Notice that all coefficients a_i in $\overline{\Psi}_h$ are positive, since $\overline{\Psi}_h$ is associated with the composition map

$$\bar{\psi}_h = \varphi_{ch}^{[B]} \circ \varphi_{b_m h}^{[B]} \circ \varphi_{a_m h}^{[A]} \circ \cdots \circ \varphi_{b_1 h}^{[B]} \circ \varphi_{a_1 h}^{[A]} \circ \varphi_{-ch}^{[B]}, \tag{28}$$

which, as previously, can be written as a composition of the first order method χ_h and its adjoint χ_h^* with coefficients $\bar{\beta}_i$:

$$\bar{\psi}_h = \chi_{\bar{\beta}_{2k} h}^* \circ \chi_{\bar{\beta}_{2k-1} h} \circ \cdots \circ \chi_{\bar{\beta}_2 h}^* \circ \chi_{\bar{\beta}_1 h} \circ \chi_{\bar{\beta}_0 h}^*, \tag{29}$$

with $\bar{\beta}_0 = \bar{\beta}_{2k} = 0$. Since the coefficient of X_3 is zero in (27), it is clear that

$$\bar{f}_{3,1} := \sum_{i=0}^{2k} \bar{\beta}_i^3 = 0. \tag{30}$$

But, as we know from the proof of Theorem 2 provided in Section 2, this condition cannot be satisfied with all coefficients a_i positive.

Similarly, if we assume that all b_i are positive then the same argument applied to the post-processor (25) leads to the same contradiction. □

In fact, the explicit expression of the effective order conditions up to order 3 can be derived in the following way. By inserting (24) in (22) and applying the BCH formula one finds

$$\begin{aligned}\widehat{\Psi}_h = \exp\bigg(& hX_1 + h^2(f_{2,1} + 2c)X_2 + h^3\bigg(\big(f_{3,1} + 3c(f_{2,1} + c)\big)X_3 \\ &+ \bigg(f_{3,2} - \frac{1}{2}c(f_{2,1} + c) + d_1\bigg)[X_1, X_2]\bigg)\bigg) + \mathcal{O}\big(h^4\big)\end{aligned} \tag{31}$$

and a second order method is obtained by taking $c = -\frac{1}{2} f_{2,1}$. If we substitute this value in (31) and take d_1 such that the coefficient of $[X_1, X_2]$ vanishes, then

$$\widehat{\Psi}_h = \exp\bigg(hX_1 + h^3\bigg(f_{3,1} - \frac{3}{4} f_{2,1}^2\bigg)X_3\bigg) + \mathcal{O}\big(h^4\big). \tag{32}$$

This same result is obtained if one considers a post-processor such that (25) holds (with $c_2 = 0$) instead of (24). In summary, it is clear that

$$f_{3,1} - \frac{3}{4} f_{2,1}^2 = 0 \tag{33}$$

is the only condition to be satisfied by a composition to be of effective order three. This condition is equivalent to the kernel condition at order three presented in [2] using a different basis of the Lie algebra.

Example. Let us consider the composition map

$$\psi_h = \varphi_{(1-b)h}^{[B]} \circ \varphi_{(1-a)h}^{[A]} \circ \varphi_{bh}^{[B]} \circ \varphi_{ah}^{[A]} = \chi_{\beta_4 h}^* \circ \chi_{\beta_3 h} \circ \chi_{\beta_2 h}^* \circ \chi_{\beta_1 h} \circ \chi_{\beta_0 h}^*, \tag{34}$$

with $\beta_0 = 0$, $\beta_1 = a$, $\beta_2 = b - a$, $\beta_3 = 1 - b$, $\beta_4 = 0$, and the consistency conditions already imposed. This composition cannot be of order three (there are not enough parameters to solve all the order conditions (9)), yet it could be of effective order three if condition (33) is satisfied, which in this case reads

$$1 - 12ab(1-a)(1-b) = 0.$$

But it turns out that this equation has no real solution if $a \in (0, 1)$ as well as if $b \in (0, 1)$.

4. Other classes of composition methods

The previous results can be generalized in different contexts. For instance, let us consider a partitioned scheme built up using finite linear combinations of splitting methods of the form (5), i.e.,

$$\psi_h = \sum_{k=1}^{K} \gamma_k \, \psi_{h,k}, \tag{35}$$

where

$$\psi_{h,k} = \varphi_{b_{k,n}h}^{[B]} \circ \varphi_{a_{k,n}h}^{[A]} \circ \cdots \circ \varphi_{b_{k,1}h}^{[B]} \circ \varphi_{a_{k,1}h}^{[A]} \tag{36}$$

and it is assumed that $\sum_k \gamma_k = 1$ and $\sum_i a_{k,i} = \sum_i b_{k,i}$, $k = 1, \ldots, K$. The generalization provided by the following theorem establishes that even with partitioned schemes of the form (35) each basic flow in a convex partition ($\gamma_k > 0$ for every $1 \leqslant k \leqslant K$) must be applied for at least one backward fractional time step. On the other hand, simple polynomial extrapolation of the leapfrog method (7) shows that if $\gamma_k < 0$ all the coefficients $a_{k,i}$, $b_{k,i}$ may indeed be positive.

Theorem 4 [9]. *If p and K are positive integers such that $p \geqslant 3$ and $K \geqslant 2$, and $\gamma_k > 0$ for $k = 1, \ldots, K$, then at least one of the coefficients $a_{k,i}$ as well as one of the $b_{k,i}$ have to be negative in the composition* (36) *if ψ_h has order, or effective order, $p \geqslant 3$.*

Proof. Also in this case the proof is quite elementary. Since $\sum_i a_{k,i} = \sum_i b_{k,i}$ we can write

$$\psi_{h,k} = \chi_{\beta_{k,2n}h}^* \circ \chi_{\beta_{k,2n-1}h} \circ \cdots \circ \chi_{\beta_{k,2}h}^* \circ \chi_{\beta_{k,1}h} \circ \chi_{\beta_{k,0}h}^* \tag{37}$$

and by following the same procedure as previously we find that instead of (16) the necessary condition for (35) to be a method of order three or higher is now

$$\sum_{k=1}^{K} \gamma_k \sum_{i=1}^{2n} \beta_{k,i}^3 = 0.$$

Since $\gamma_k > 0$, $k = 1, \ldots, K$, there exists some j, $1 \leqslant j \leqslant K$, such that

$$\sum_{i=1}^{2n} \beta_{j,i}^3 \leqslant 0,$$

and the previous proof can be applied. □

The two-term splitting analyzed so far can be seen as a special instance of a k-term splitting of the vector field F, $F = F_1 + F_2 + \cdots + F_k$. Suppose we have a scheme of the form

$$\begin{aligned}\psi_h = {} & \varphi_{a_{m,k}h}^{[k]} \circ \cdots \circ \varphi_{a_{m,2}h}^{[2]} \circ \varphi_{a_{m,1}h}^{[1]} \circ \cdots \circ \varphi_{a_{2,k}h}^{[k]} \circ \cdots \circ \varphi_{a_{2,2}h}^{[2]} \circ \varphi_{a_{2,1}h}^{[1]} \\ & \circ \varphi_{a_{1,k}h}^{[k]} \circ \cdots \circ \varphi_{a_{1,2}h}^{[2]} \circ \varphi_{a_{1,1}h}^{[1]},\end{aligned} \tag{38}$$

where $\varphi_h^{[l]}$ stands for the exact h-flow of the vector field F_l. If the composition (38) is of order, or effective order, $p \geqslant 3$ for all choices of operators $F_1, \ldots, F_k$, then clearly

$$\min_{1 \leqslant i \leqslant m} a_{i,l} < 0, \quad l = 1, \ldots, k.$$

Consider now composition maps of the Strang splitting $\psi_{h,2}$ given by (4) (or with the roles of the flows $\varphi_h^{[A]}$ and $\varphi_h^{[B]}$ interchanged), i.e.,

$$\psi_h = \psi_{\beta_m h,2} \circ \psi_{\beta_{m-1}h,2} \circ \cdots \circ \psi_{\beta_1 h,2} \circ \psi_{\beta_0 h,2}. \tag{39}$$

The series of differential operators S_h associated with the integrator $\psi_{h,2}$, i.e., such that $g \circ \psi_{h,2} = S_h[g]$, can be written as $S_h = \exp(X_h)$, where $X_h = hX_1 + h^3 X_3 + h^5 X_5 + \cdots$, $X_1 = F$ and

$$\Psi_h = \exp(X_{\beta_0 h}) \exp(X_{\beta_1 h}) \cdots \exp(X_{\beta_{m-1} h}) \exp(X_{\beta_m h}).$$

Now, by repeated application of the BCH formula,

$$\Psi_h = \exp\bigl(h f_{1,1} X_1 + h^3 f_{3,1} X_3 + \mathcal{O}\bigl(h^4\bigr)\bigr),$$

where

$$f_{1,1} = \sum_{i=0}^{m} \beta_i, \qquad f_{3,1} = \sum_{i=0}^{m} \beta_i^3.$$

Therefore $f_{1,1} = 1$, $f_{3,1} = 0$ are necessary conditions for ψ_h to be of order $p \geqslant 3$. In fact, since $f_{2,1} = 0$ in this case, they are also the conditions to be satisfied by ψ_h to have effective order $p = 3$ and the following theorem can be established.

Theorem 5. *If p is any positive integer such that $p \geqslant 3$ and $\psi_{h,2}$ is the Strang splitting* (*or Störmer/Verlet scheme*) (4), *then at least two consecutive coefficients a_i, b_i have to be negative in the composition* (39) (*when it is expressed in terms of the basic flows $\varphi_h^{[A]}$, $\varphi_h^{[B]}$*) *if ψ_h is of order, or effective order, p. Even more, at least two coefficients a_{i_1}, a_{i_2} have to be negative.*

Proof. By substituting in (39) the expression of the basic method $\psi_{\beta_i h,2} = \varphi_{\beta_i h/2}^{[A]} \circ \varphi_{\beta_i h}^{[B]} \circ \varphi_{\beta_i h/2}^{[A]}$, we obtain a composition of the type (5) with

$$b_i = \beta_i, \qquad a_i = \frac{1}{2}(\beta_i + \beta_{i-1}), \quad i = 1, \ldots, m, \tag{40}$$

if $\beta_0 = \beta_m = 0$. It is immediate to check that if there exists one negative coefficient, say $\beta_j < 0$, $1 \leqslant j \leqslant m-1$, and

$$|\beta_j| > \beta_{j-1}, \tag{41}$$

then $a_j < 0$, $b_j < 0$, whereas if

$$|\beta_j| > \beta_{j+1}, \tag{42}$$

then $b_j < 0$, $a_{j+1} < 0$. In other words, as soon as one of the β_i is negative and its absolute value is higher than the previous one or the next one then the corresponding composition (5) has, at least, two consecutive coefficients which are negative.

Let us analyse the different possibilities arising from the order condition $f_{3,1} = 0$.

(i) First, suppose there exists only one negative coefficient $\beta_j < 0$, $1 \leqslant j \leqslant m-1$. Then

$$\beta_j = -\left(\sum_{i \neq j} \beta_i^3\right)^{1/3}$$

and both conditions (41) and (42) are satisfied so that, according to the previous discussion, $a_j < 0$, $b_j < 0$ and $a_{j+1} < 0$.

(ii) Suppose now that there are $k \geqslant 2$ negative coefficients, $\beta_{j_1}, \beta_{j_2}, \ldots, \beta_{j_k} < 0$ such that they do not satisfy conditions (41) and (42). Observe that they cannot be consecutive, otherwise either (41) or (42) are satisfied. Then we can write condition $f_{3,1} = 0$ as

$$\beta_{j_k} = -\Big(\big(\beta_{j_1-1}^3 + \beta_{j_1}^3\big) + \cdots + \big(\beta_{j_{k-1}-1}^3 + \beta_{j_{k-1}}^3\big) + \sum{}' \beta_i^3\Big)^{1/3},$$

where $\sum'$ contains the remaining terms, including β_{j_k-1} and β_{j_k+1}. Since $\beta_{j_i-1}^3 + \beta_{j_i}^3 > 0$, $i = 1, \ldots, k-1$, then $\beta_{j_k-1} < |\beta_{j_k}|$, $\beta_{j_k+1} < |\beta_{j_k}|$, conditions (41) and (42) are in fact satisfied by β_{j_k} and therefore $b_{j_1}, \ldots, b_{j_k-1}, a_{j_k}, b_{j_k}, a_{j_k+1} < 0$.

(iii) Finally, consider the case in which $\beta_{j_1}, \beta_{j_2}, \ldots, \beta_{j_k} < 0$ ($k \geqslant 2$) and only one of the coefficients β_{j_i}, $i = 1, \ldots, k$, satisfies either (41) or (42). For instance, suppose that β_{j_1} is such that $|\beta_{j_1}| > \beta_{j_1-1}$ (and therefore $a_{j_1} < 0$). Then, condition $f_{3,1} = 0$ can be expressed as

$$\big(\beta_{j_1}^3 + \beta_{j_1+1}^3\big) + \sum_{i \neq j_1, j_1+1} \beta_i^3 = 0,$$

but $\beta_{j_1}^3 + \beta_{j_1+1}^3 > 0$, since (42) is not satisfied by β_{j_1}, so that

$$\big(\beta_{j_2}^3 + \beta_{j_2+1}^3\big) + \cdots + \big(\beta_{j_k}^3 + \beta_{j_k+1}^3\big) + \sum{}' \beta_i^3 < 0,$$

where, as before, $\sum'$ contains the remaining (positive) terms. In consequence, there must exist some $2 \leqslant i \leqslant k$ such that $\beta_{j_i}^3 + \beta_{j_i+1}^3 < 0$. Therefore we have at least $b_{j_1}, \ldots, b_{j_k} < 0$ and $a_{j_1}, a_{j_i+1} < 0$.

If β_{j_1} satisfies (42) instead, a similar strategy applies and the same conclusion follows. □

This result, together with the discussion of Section 2 justifies why it is so frequent that at least two consecutive coefficients are negative.

5. Composition methods with all coefficients being positive

Let us consider now the second order differential equation

$$y'' = g(y), \tag{43}$$

which can be written in the form (1) by taking $x \equiv (x_1, x_2) = (y, y')$ and $f_A(x) = (x_2, 0)$, $f_B(x) = (0, g(x_1))$, or equivalently

$$F_A \equiv x_2 \frac{\partial}{\partial x_1}, \qquad F_B \equiv g(x_1) \frac{\partial}{\partial x_2}.$$

This equation frequently appears in relevant problems arising in classical and quantum mechanics: there the operator F_A is related to the kinetic energy (quadratic in momenta) and F_B is associated with the potential energy. Now the flow corresponding to $F_C \equiv [F_B, [F_A, F_B]]$ is explicitly and exactly computable and, in addition, $[F_B, F_C] = 0$, so that it makes sense to compute the 1-flow $\varphi^{[B,C]}_{bh,ch^3}$ associated with the vector field $hbF_B + ch^3 F_C$ and include it into the composition (5):

$$\psi_h = \varphi^{[B,C]}_{b_m h, c_m h^3} \circ \varphi^{[A]}_{a_m h} \circ \cdots \circ \varphi^{[B,C]}_{b_1 h, c_1 h^3} \circ \varphi^{[A]}_{a_1 h}. \tag{44}$$

In this case ψ_h cannot always be written as the composition of a first order scheme and its adjoint, and Theorem 2 does not necessarily apply. For instance

$$\psi_h = \varphi^{[B]}_{h/6} \circ \varphi^{[A]}_{h/2} \circ \varphi^{[B,C]}_{2h/3, h^3/72} \circ \varphi^{[A]}_{h/2} \circ \varphi^{[B]}_{h/6} \tag{45}$$

is a method of order four [11] and

$$\psi_h = \varphi^{[A]}_{h/2} \circ \varphi^{[B,C]}_{h, h^3/24} \circ \varphi^{[A]}_{h/2} \tag{46}$$

is a method of effective order four [19]. In the last case we can write $\psi_h = \chi^*_{h/2} \circ \chi_{h/2}$ with $\chi_h \equiv \varphi^{[B,C]}_{h,h^3/6} \circ \varphi^{[A]}_h$. However, if we analyse the corresponding operator $\exp(X_h) = \exp(hX_1 + h^2 X_2 + h^3 X_3 + \cdots)$ associated with χ_h, we find that $X_3 = [X_1, X_2]/6$. Then X_3 is not an independent element and its contribution can be cancelled with a proper choice of the map π_h, thus giving a fourth-order method.

Numerical experiments suggest that this is the highest order one can get with the composition (44) with positive coefficients and a rigorous proof is at present under investigation. However, methods of effective order six as well as of order six are known to exist with all coefficients b_i being positive.

On the other hand, if we consider a Hamiltonian system of the form

$$H = T(p) + V(q),$$

with T quadratic in p and $V(q)$ a polynomial function up to degree four in q (or, in general, if $g(y)$ is a polynomial function up to degree three), then $F_E \equiv [F_A, [F_A, [F_A, [F_A, F_B]]]]$ vanish or depends only on the momenta, i.e., $[F_A, F_E] = 0$, and its flow can be computed exactly. In addition $F_D \equiv [F_B, [F_B, [F_A, [F_A, F_B]]]]$ depends only on the coordinates and thus $[F_B, F_D] = 0$. Thus one may consider composition maps involving the 1-flows $\varphi^{[A,E]}_{ah,eh^5}$, $\varphi^{[B,C,D]}_{bh,ch^3,dh^5}$ corresponding to the vector fields $haF_A + eh^5 F_E$ and $hbF_B + ch^3 F_C + dh^5 F_D$, respectively. In particular, the generalised leapfrog splitting scheme

$$\psi_h = \varphi^{[A,E]}_{h/2,eh^5} \circ \varphi^{[B,C,D]}_{h,ch^3,dh^5} \circ \varphi^{[A,E]}_{h/2,eh^5}, \tag{47}$$

with $c = \frac{1}{24}$, $d = \frac{1}{1440}$, $e = \frac{1}{2880}$ is a method of effective order six, since these coefficients satisfy the kernel conditions collected in [2] up to this order.

We should recall that methods (45)–(47) are particular examples of composition schemes involving only positive coefficients. The possible existence of other families of composition methods of order $p \geqslant 3$ with positive coefficients is, at the time being, an open question of great interest, for instance, in the numerical integration of nonreversible systems.

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Since the completion of this work, S.A. Chin has published a different proof of Theorem 3; see [5].

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